AD-763 496

ELECTRONIC STATES IS DISORDERED
MATERIALS

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Prepared for:

Army Research Office-Durham
Advanced Research Projects Agency

31 January 1973

Semi-Annual Technical Report

August 1, 1972 to January 31, 1973

ARPA Order No. 1562

Profram Code No. OD10

Name of Grantee
University of North Carolina at
    Chapel Hill

Effective date of Grant
    April 1, 1972

Expiration Date
    March 31, 1973

Amount of Grant
    $32,892

Grant No.
DA-ARCD-31-124-71-G52

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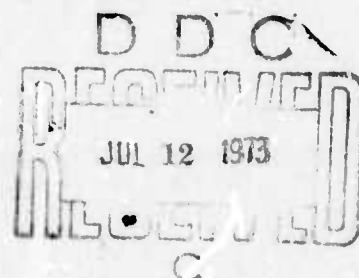
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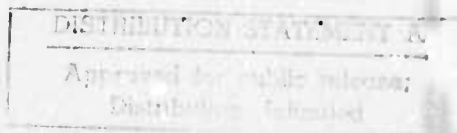Short Title: Electronic States
is Disordered Materials

AD 763496

Sponsored by

Advanced Research Projects Agency

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Theory

The tight-binding approach to calculating the density of states
in amorphous covalently bonded semiconductors has proven quite fruitful
in increasing our understanding of the effect of topological disorder
on the energy levels distribution in these materials. In Table 1 and
Figure 1, we summarize our results on the density of state based on the
hamiltonian

$$H = \sum_{\substack{ij \\ i \neq j}} |\phi_i\rangle\langle\phi_j| \ . \tag{1}$$

ϕ_i is the orbital associated with site i and the sum over i,j is over
nearest neighbors. These results are contained in the thesis of J. C.
Wang, a graduate student working on the problem. The Hamiltonian (1)
is also referred to in the literature as the "connectivity matrix".
Table I is the computer results for the first ten moments of the density
of states in the diamond lattice, the Polk model, the Henderson-Herman
model, and Ge III. The deviations in the moments of the various models
from that of the perfect diamond lattice demonstrate the degree of
topological disorder present. On this basis, it is interesting to observe
that the Polk and Henderson models although constructed quite differently
are not very different topologically. Figure I shows the density of states
calculated by using Montroll's method of moment inversion. Again the
result for the Polk and Henderson models are not significantly different.

Ge III is topologically different from the other models and the difference shows up in the extra peak in the density of states. This result is in accord with that calculated by J. D. Joannoponlos and M. L. Cohen using an empirical pseudo-potential method (Phys. Letters, 41A, 71 (1972)).

The tight-binding approach has demonstrated the importance of topological effects on the density of states in amorphous system. However, the effects of including more than nearest neighbor overlaps is not known, specially for states near the gap edges. In addition the method fails to produce the states at the top of the valence band correctly. On the other hand, multiple scattering calculations on clusters of scatterers up to 30 carbon atoms in size by Keller and Ziman (J. Non-Cryst. Solids, 8-10, 111 (1972)) seems to be able to give good results for states at the gap edges. The calculation is however very sensitive to the boundary conditions imposed on the clusters and are therefore inconclusive. We propose a new free-electron network model which includes the essential points of both the tight-binding and multiple scattering theories. (A similar idea was proposed independently by W. John (Phys. Stat. Sol. (b) 55, 801 (1973)), but our approach is slightly different). The multiple scattering theory by Lloyd (Proc. Phys. Soc. 90, 207 (1967) gives for the integrated density of states for a system with volume V, atomic positions $\vec{r}_i$, and atomic phase shifts δ_ℓ:

$$N(E) = \frac{E^{3/2}}{3\pi 2} - \frac{2}{\pi V} \text{ Im Tr } \ln (D) \tag{2}$$

$$= N_o(E) - \frac{2}{\pi V} \text{ Im } \ln ||D||$$

where

$$||D|| = ||\delta_{L_1 L_2} \delta_{ij} + G^+_{L_1 L_2}(\vec{r}_i - \vec{r}_j) k_{L_2}(E)|| \quad ,$$

$$G^+_{L_1 L_2}(\vec{R}) = \begin{cases} -i\sum_{L_3} 4\pi\, i^{\ell_2 + \ell_3 - \ell_1}\, C(L_1 L_2 L_3)\, h^+_{L_3}(\sqrt{E}R)\, Y_{L_3}(\hat{R}), & \vec{R}\neq 0 \\ -1\, \delta_{L_1 L_2} \quad , & \vec{R}=0 \end{cases} \tag{2}$$

$$C(L_1 L_2 L_3) = \int Y_{L_1}(\Omega) Y_{L_2}(\Omega) Y_{L_3}(\Omega)\, d\Omega \quad ,$$

and

$$k_\ell = \tan \delta_\ell \quad .$$

Because of the central role played by the connectivity matrix in our tight-binding calculation, we propose in our model to retain in (2) only those terms related by the connectivity matrix. In addition we shall assume an effective S-wave phase shift $\delta^*_o(E)$. Under these assumptions we find for the density of states,

$$dN(E)/dE = \frac{E^{\frac{1}{2}}}{2\pi^2} + \frac{2}{\pi v}\left[-\frac{a}{2\sqrt{E}}\int n(x)dx\, \frac{(x+s) + t/(\sqrt{E}a)}{(x+s)^2 + t^2} \right.$$

$$\left. + k^{*'}_o\, \frac{\sqrt{E}a}{k^{*2}_o}\, \sin\sqrt{E}a \int n(x)dx\, \frac{x+\sqrt{E}a/\sin\sqrt{E}a}{(x+s)^2 + t^2} \right] \quad , \tag{3}$$

where a is the nearest neighbor distance, $k_o^* = \tan \delta_o^*$,

$$s = \sqrt{\bar{E}}a \; (\sin\sqrt{\bar{E}}a - \cos\sqrt{\bar{E}}a/k_o^*) \quad ,$$

$$t = \sqrt{\bar{E}}a \; (\cos\sqrt{\bar{E}}a + \sin\sqrt{\bar{E}}a/k_o^*) \quad ,$$

and $n(x)$ is the density of states of (1) as shown in Figure 1.

In Eq. (3), the second and third terms will be sensitive to the topology through $n(x)$ if t were small. When t is large the result becomes sensitive to $k_o'(E)$. We believe that in amorphous Ge and Si, t will be small for the range of energy at the lower half of the valence band and hence topological disorder will dominate this part of the density of states. For energy at the top of the valence band, t will be large and the energy dependence of $k_o(E)$ will begin to dominate. This theory seems to be extremely promising in providing a simple way of understanding the energy levels distribution in amorphous materials. The results reported here are preliminary. We are at present involved in trying to justify our assumptions rigorously.

Our experimental result during this period are briefly summarized in Figure 2. Figure 2 shows some typical results of mobility versus density for various temperatures. Included are some data taken at 20°K which go out to densities of 5×10^{21} cm^{-3}. The comparison of the 20°K data and the 77°K data is sticking. It is one of the few examples we know of where a decrease in temperature at say 3.5×10^{21} cm^{-3} results in a very large increase in mobility. It is primarily this comparison that leads us to the presumption that at 77°K the low mobility branch is due to self trapped electrons and that self trapping is thermally activated. (The 20°K data shows transport in

the band tail states and so one gets a single unique mobility similar to the 4.2°K results).

The trapping effect seen at 77°K by the two branches is inferred from the fact that two branches represent non-equilibrium between a low mobility and a high mobility state. The magnitude of the signals depends upon the transit time of the free carriers and the density as one would expect in a transient trapping situation. Figure 3 shows the magnitude of the high and low mobility signals as a function of density. One should notice how rapidly the low mobility signal increases with density. At any density the magnitude of this signal should be $i = i_0 [1 - \exp(-t/\tau)]$ where τ is the trapping time. If the trapping were due to impurities (which are frozen out at 77°K) then one would expect τ to vary as the reciprocal of the density). Figure 4 shows how τ varies with density and one sees that the decrease in τ is much faster than the reciprocal of the density. Also shown is the life time for thermalization of hot electrons. Indeed this time does depend up the reciprocal of the density at least at the densities where double branching is seen. We believe that these results imply the density of available self trapped states and possible the activation energy for populating these states is density dependent.

TABLE I . The first ten moments of the one-band density of
states of the perfect diamond lattice, Polk model,
Henderson-Herman model, and Ge III. The result of the Polk
model is the average over the center 33 atoms.

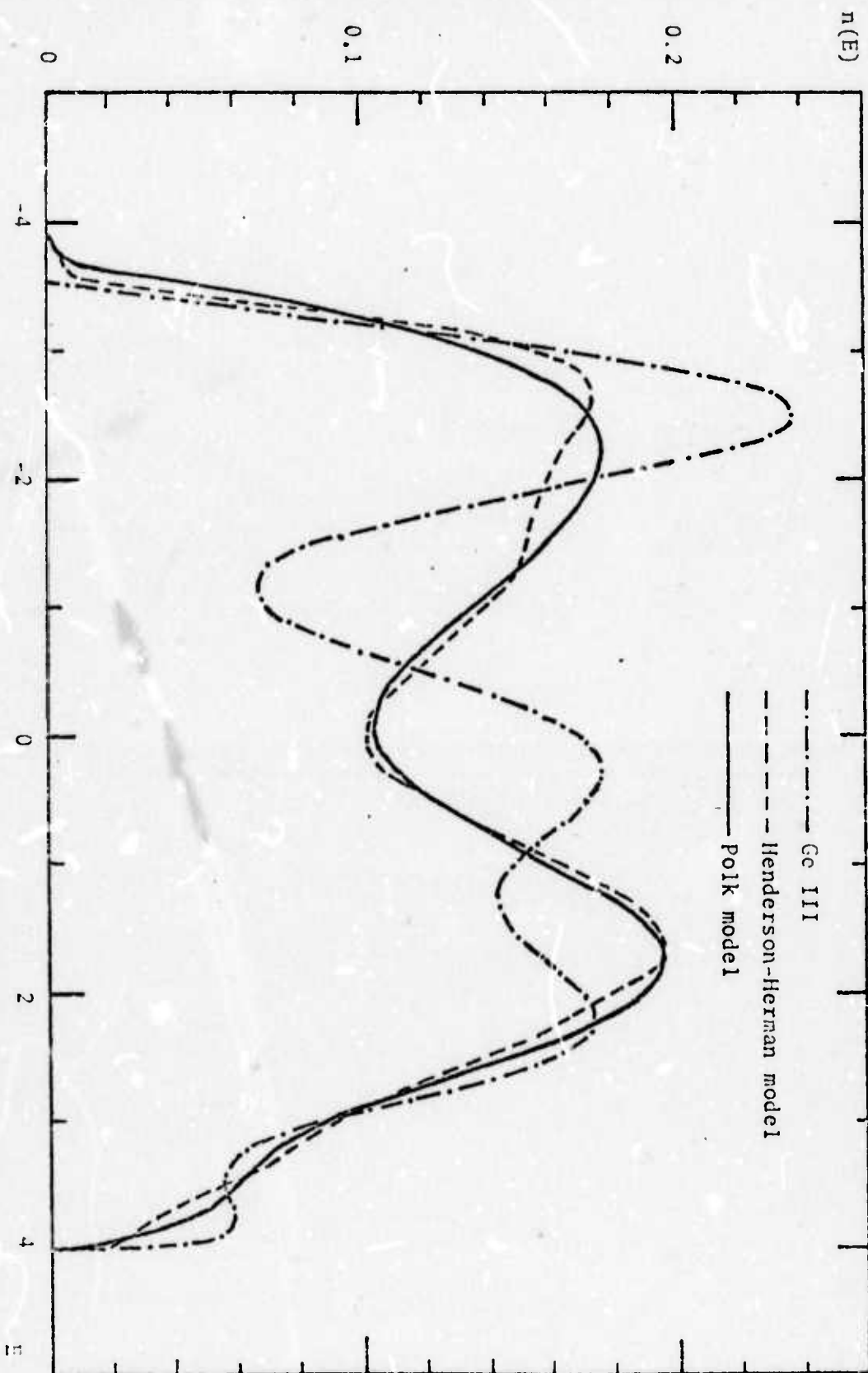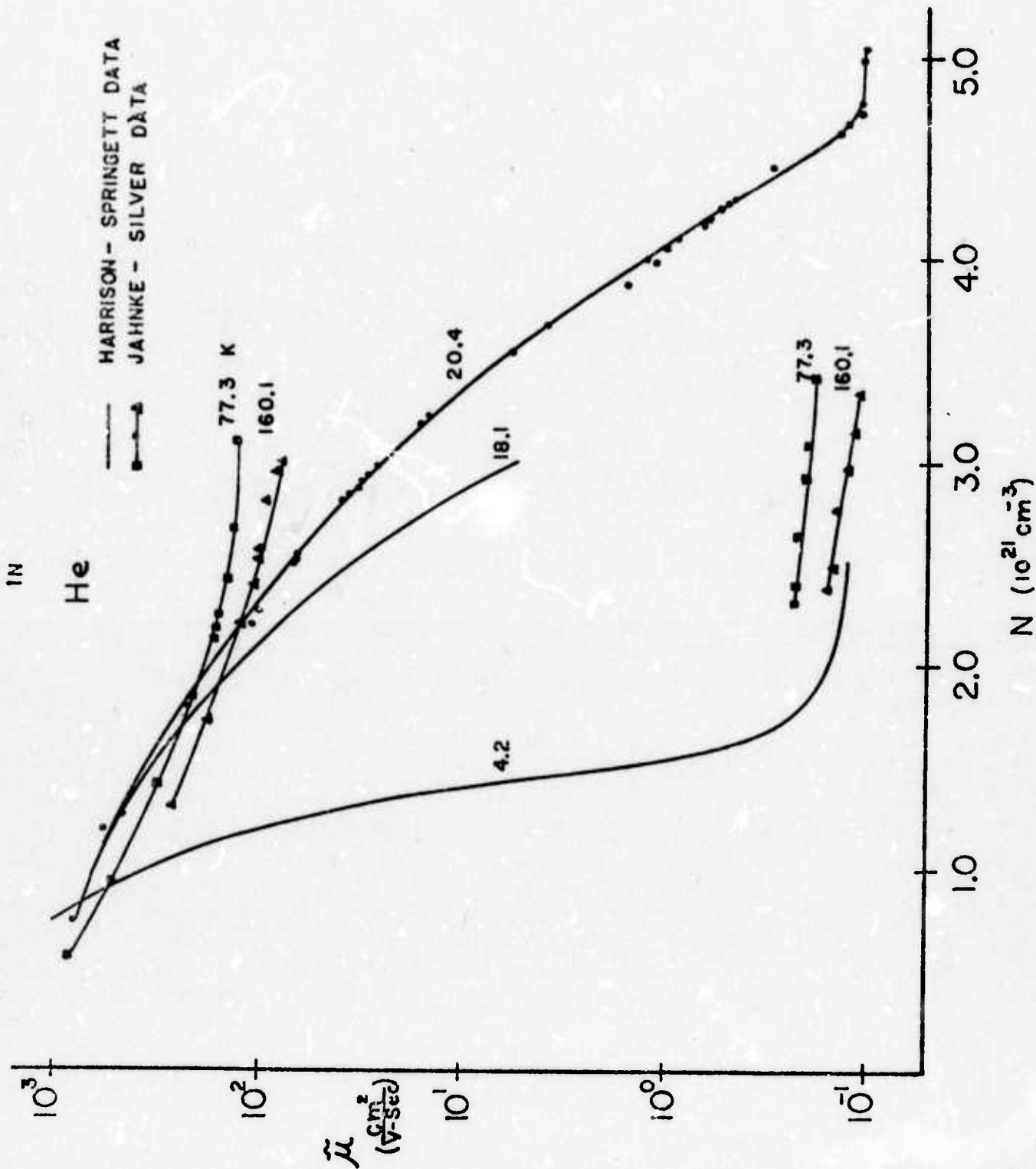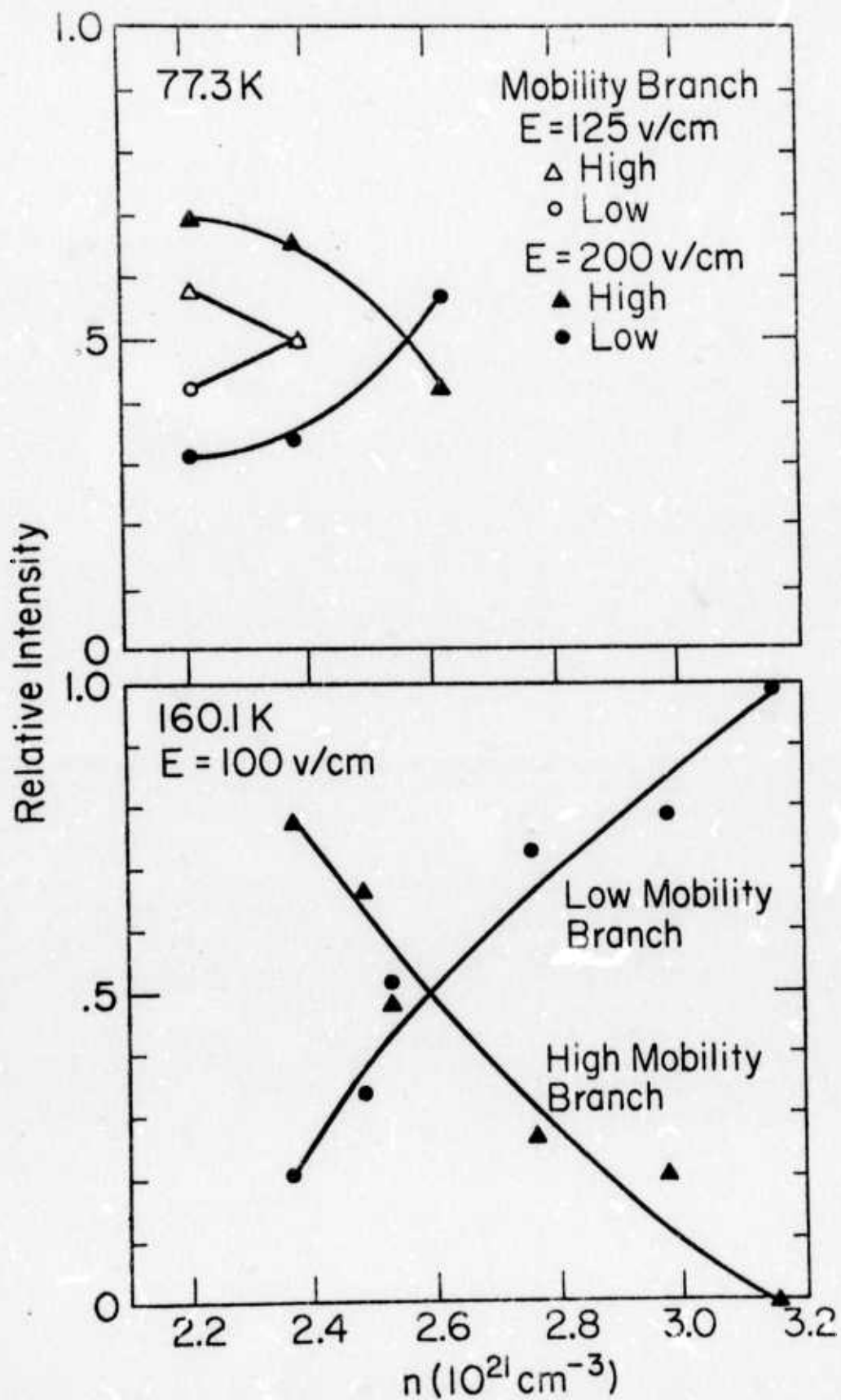|	Perfect	Polk	Henderson	Ge III
M_0	1	1	1	1
M_1	0	0	0	0
M_2	4	4	4	4
M_3	0	0	0	0
M_4	28	28	28	28
M_5	0	3.5151	4.0984	6.6667
M_6	256	244.3636	242.8197	236
M_7	0	86.3636	100.9836	149.3333
M_8	2716	2419.0909	2379.7377	2241.3333
M_9	0	1561.8788	1821.2459	2436
M_{10}	31504	25990.6667	25333.6721	23257.3333

Fig. 1. n(E) curves calculated with the first ten moments for the Polk model, Henderson-Herman model and Ge III.

ELECTRON MOBILITY VS NUMBER DENSITY IN He

HARRISON - SPRINGETT DATA
JAHNKE - SILVER DATA

Physlet A 1096 fig 2

τ_{th} + $\tau_{S.T.}$ vs DENSITY